

Decoherence and localization in the double well model

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Abstract

We use a spin-1/2 model to analyze tunnelling in a double well system coupled to an external reservoir. We consider different noise sources such as fluctuations on the height and central position of the barrier and propose an experiment to observe these effects in trapped ions or atoms.

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Tunnelling is a purely quantum phenomenon where a trapped massive particle escapes from the trapping potential even though its total energy is smaller than the trapping barrier itself. This mechanism is another manifestation of

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interference in quantum mechanics. It is also the origin of delocalization in many different quantum systems.

For example, consider a particle trapped in a symmetric double well potential, and consider it initially localized in the left side of the barrier. According to classical mechanics, if the energy of the particle is smaller than the energy of the middle barrier, the particle will remain on the left side forever. Quantum mechanics, however, predicts that if the barrier is not infinite, then there is a non-null probability that the particle will eventually tunnel to the right side of the trap. In fact, if the whole system is isolated, and the particle is in a low-energy level, the dynamics of this trapped particle will present oscillations between the localized states to the left and right of the middle barrier and in general the particle will be delocalized in the two sides of the barrier.

On the other hand, we also know that interference of quantum states can be irreversibly destroyed when the corresponding system interacts and entangles with much larger ones, so-called reservoirs, in a quantum effect known as decoherence. This effect has been widely studied in many different systems and it has helped the comprehension of fundamental questions such as localization and the quantum-classical transition [1], [2], [3], [4], [5], [6].

In this paper we study the problem of tunnelling, decoherence and localization in the double well potential. We were motivated by the question of finding a simple qualitative model to determine the effect of the coupling of a quantum system, able to undergo tunnelling between two potential wells, to dissipative degrees of freedom. We map our problem into that of a spin 1/2 particle coupled to a classical static magnetic field and subjected to spin-flip and dephasing reservoirs. We show how this noise ends up localizing the particle in one side of the barrier, and we propose an experiment to observe these effects on trapped ions or atoms.

The manuscript is organized as follows: first, we map out the movement of the center of mass of the trapped particle into a spin-1/2 problem. Then we describe the dynamics of this fictitious spin-1/2 when subjected to different noise sources to which we associate fluctuations in the position and height/width of the separating potential barrier. Finally, we suggest an experiment to observe this dynamics in trapped ions.

Let us consider a particle in a symmetric double well potential, i.e. an infinite one-dimensional well ($V(-x_{max}) = V(x_{max}) = \infty$) with a finite potential barrier in the center ($0 < V(0) = V_0$). Due to the symmetry of this configuration, the eigenstates of this confining Hamiltonian can be either even (symmetrical) or odd (antisymmetrical) functions. Consider the central potential barrier very high; the arrangement can be looked upon as two infinite potential wells. In such a case each possible energy value is twofold degenerate. When the

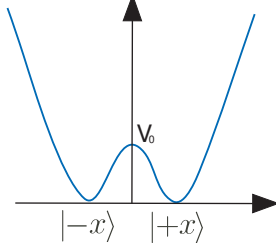


Fig. 1. The symmetric double well. We associate each side of the potential barrier through which the particle can tunnel with the eigenstates of the S_x component of the spin.

finite height of the potential barrier is taken into account, the tunnel effect across the barrier removes the degeneracy, and the first levels splits, giving rise to doublets $\{|n_s\rangle, |n_a\rangle\}$ (s for symmetrical, a for antisymmetrical), with respective energies E_{n_s} and E_{n_a} . The large barrier assumption can be written $E_{n_s}, E_{n_a} \ll V_0$ for small n . It also implies $|E_{n_s} - E_{n_a}| \ll |E_{n+1_s} - E_{n_s}|$, i.e. the energy separation between neighbor doublets is much larger than their splitting. This allows us to treat each doublet as a separate two-level system.

From now on, we will consider only the first doublet and represent it as a spin-1/2 particle precessing around an uniform classical magnetic field in a fictitious spin picture [7]. There are infinite equivalent ways of building this analogy. We will choose to associate each side of the potential barrier with the eigenstates $|-x\rangle$ (left side of the barrier) and $|+x\rangle$ (right side of the barrier) of the S_x component of this spin. In this case, the symmetrical and antisymmetrical stationary states in the well, given by $|s\rangle = \frac{|+x\rangle + |-x\rangle}{\sqrt{2}}$ and $|a\rangle = \frac{|+x\rangle - |-x\rangle}{\sqrt{2}}$, will be associated with the eigenstates of S_z ($\sigma_z = |s\rangle\langle s| - |a\rangle\langle a|$). The back and forth motion of the particle through the potential barrier inside the well can be associated with the precession of this fictitious spin-1/2 around an uniform magnetic field parallel to the O_z axis, with frequency $\omega = \frac{|E_{0_s} - E_{0_a}|}{\hbar}$. This oscillation can also be viewed as a succession of constructive and destructive interference of the symmetrical and antisymmetrical wavefunctions. The dynamics of this isolated system is then described by the Hamiltonian $H = -\frac{\omega}{2}\sigma_z$.

Considered as an open quantum system, the dynamics of this virtual two-level particle is better described by the following Lindblad master equation [8](in units of $\hbar = 1$):

$$\dot{\rho} = -i\frac{\omega}{2}[\sigma_z, \rho] - \frac{1}{2} \sum_{k=1}^n \{\Gamma_k^\dagger \Gamma_k \rho + \rho \Gamma_k^\dagger \Gamma_k - 2\Gamma_k \rho \Gamma_k^\dagger\}, \quad (1)$$

with each Γ_k being associated to a different decohering process.

Continuing our analogy, we can associate random fluctuations of the height or width (with symmetry preservation) of the barrier to a phase reservoir

in the spin system represented by $\Gamma_1 = \sqrt{k_1}\sigma_z$. We justify this equivalency by the following argument: small fluctuations in the height or width of the barrier (i.e. vertical or horizontal symmetric shaking of the barrier) do not change the eigenstates of the barrier, but only result in small fluctuations in ω , causing dephasing between the symmetrical and antisymmetrical states, which characterizes a phase reservoir. In the magnetic field analogy, this corresponds to fluctuations on B_z , but keeping $B_x = B_y = 0$.

Another decoherence source can be associated with fluctuations of the position of the barrier. Small shifts around the central position of the barrier result in new eigenstates for the system. Those can be obtained as linear combinations of the former ones, and the whole process can be described as a small B_x fluctuation, for example. We can therefore associate this phenomenon with a spin flip reservoir described by $\Gamma_2 = \sqrt{k_2}\sigma_x$.

We first consider only the phase reservoir Γ_1 , i.e. the shaking of the potential barrier in the well. The master equation describing the evolution of the system becomes:

$$\dot{\rho} = -i\frac{\omega}{2}[\sigma_z, \rho] - k_1\{\rho - \sigma_z\rho\sigma_z\}, \quad (2)$$

since $\sigma_z = \sigma_z^\dagger$ and $\sigma_z^2 = \mathbb{I}$. To solve the above master equation we consider the Bloch vector parametrization

$$\rho(t) = \frac{1}{2} \begin{pmatrix} 1 + S_z(t) & S_x(t) + iS_y(t) \\ S_x(t) - iS_y(t) & 1 - S_z(t) \end{pmatrix}, \quad (3)$$

with general pure state initial condition (spin in an arbitrary direction)

$$\rho(0) = \frac{1}{2} \begin{pmatrix} 1 + \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & 1 - \cos\theta \end{pmatrix}. \quad (4)$$

The equations of motion for S_x , S_y , and S_z obtained are:

$$\begin{aligned} \dot{S}_x &= -2k_1 S_x + \omega S_y, \\ \dot{S}_y &= -\omega S_x - 2k_1 S_y, \\ \dot{S}_z &= 0. \end{aligned} \quad (5)$$

As one should expect, the phase reservoir preserves the S_z component of the spin, which means that the eigenstates of S_z are stationary solutions of equation (2). In general, the solution to the master equation (2) is given by

$$\begin{aligned}
S_x(t) &= e^{-2k_1 t} (A \cos \omega t + B \sin \omega t), \\
S_y(t) &= e^{-2k_1 t} (-A \sin(\omega t) + B \cos(\omega t)), \\
S_z(t) &= C,
\end{aligned} \tag{6}$$

with the constants A , B and C determined by the initial state. The time dependent density matrix is then given by

$$\rho(t) = \frac{1}{2} \begin{pmatrix} 1 + \cos \theta & e^{-i\phi} \sin \theta e^{-2(k_1 + i\omega)t} \\ e^{i\phi} \sin \theta e^{-2(k_1 - i\omega)t} & 1 - \cos \theta \end{pmatrix}. \tag{7}$$

For example, let us consider an initial state $|+x\rangle$ ($\theta = \pi/2$ and $\phi = 0$), which corresponds to an even superposition of the symmetrical and antisymmetrical eigenstates of the barrier. In this case, the particle is initially localized in the left side of the barrier. Note, however, that this localization should be viewed as constructive interference of the symmetric and antisymmetric solutions of the trapping potential. Also note that, once the system evolves in time, the particle will tunnel through the barrier and the probability to find it on the left will be given by

$$P_l(t) = \frac{1}{2} [1 + e^{-2k_1 t} \cos(\omega t)]. \tag{8}$$

The above probability shows that the particle undergoes quantum dissipative oscillations between both sides of the barrier, but, asymptotically tends to localize, now in the classical statistical sense, with equal probabilities $P_l(\infty) = P_r(\infty) = 1/2$, either to the left or the right of the central barrier. By classical localization we mean that the initial pure state turns into a statistical mixture, i.e. it is no longer possible to observe interference in the system

We can also observe this classical localization by calculating the purity of the system as a function of time, which, for two level systems, can be defined by

$$\zeta(t) = 2\text{tr}\rho(t)^2 - 1. \tag{9}$$

This quantity varies from zero, for the completely random state, to one, for pure states. In fact, it gives the squared norm of the Bloch vector. From Eq. (7), one obtains

$$\zeta(t) = e^{-4k_1 t}, \tag{10}$$

which confirms that the quantum state of the particle evolves from a pure state ($\zeta(0) = 1$) to a classically localized state ($\zeta(t \gg 1/k_1) \rightarrow 0$) due to the action of the external reservoir.

Also note that for an arbitrary angle θ , the density matrix for $t \gg k_1$ tends again to a mixture of states $|+_z\rangle$ and $|-_z\rangle$, but now with different populations.

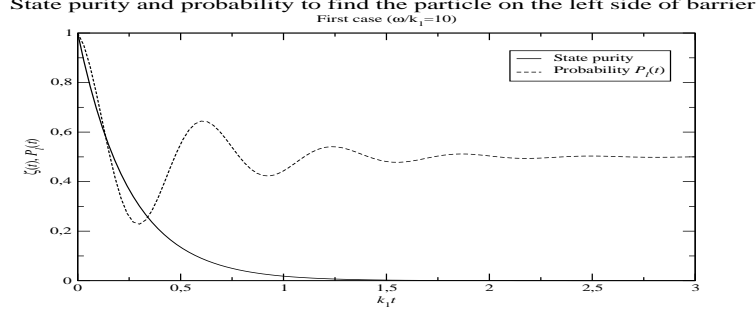


Fig. 2. The tunnelling system coupled to the σ_z reservoir: state purity $\zeta(t)$ and probability to find the particle in the left side of the double well $P_l(t)$ as a function of time, when the particle is initially prepared in the same left side ($\theta = \frac{\pi}{2}$ and $\phi = 0$) and for $k_1 = 1$ and $\omega = 10$. Note that the purity of the system tends to zero, indicating loss of coherence, and the probability tends to one-half, thus indicating localization.

$$\rho(t \rightarrow \infty) = \frac{1}{2} \begin{pmatrix} 1 + \cos \theta & 0 \\ 0 & 1 - \cos \theta \end{pmatrix}. \quad (11)$$

This result should be expected given that the phase reservoir affects only the coherence of the quantum state, i.e. it preserves the original populations of the quantum state in the σ_z basis.

A Bloch sphere picture allows a simple visual comprehension of these effects (see figure 3). First, one should remember that a Bloch vector only describes density operators. It can be thought of as an ensemble average on pure state realizations. The isolated and initially pure system would imply circular trajectories with constant z component and constant angular velocity. The phase reservoir induces velocity fluctuations. The ensemble then spreads over the circle, and the x and y components of the Bloch vector decay exponentially. For long times (compared to k_1^{-1}) the vector will be very close to the projection of the initial state onto the O_z axis.

It is interesting to notice that two special states are not affected by this reservoir. The $|+_z\rangle$ and $|-_z\rangle$ states can be viewed as rigorous pointer states [9] since they never lose purity.

Next we consider only the spin-flip reservoir, which corresponds to fluctuations of the position of the barrier inside the potential well (i.e. an asymmetric disturbance). The corresponding master equation is given by:

$$\dot{\rho} = -i\frac{\omega}{2}[\sigma_z, \rho] - k_2\{\rho - \sigma_x \rho \sigma_x\}, \quad (12)$$

since $\sigma_x = \sigma_x^\dagger$ and $\sigma_x^2 = \mathbb{I}$. In this case, the equations of motion for S_x , S_y and S_z are:

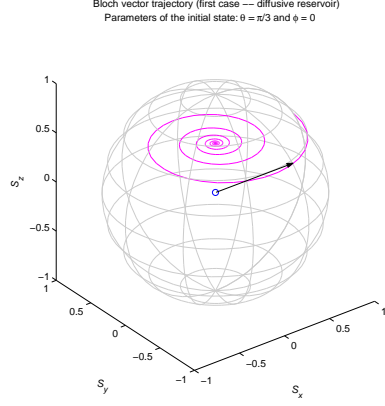


Fig. 3. A schematic diagram of the Bloch vector evolving in the Bloch sphere for an arbitrary initial state defined by the angles θ and ϕ . Only the x and y components of the Bloch vector are affected by the reservoir. On the other hand, the z component is preserved and, in the asymptotic limit, the Bloch vector tends to the projection of the initial state on the O_z axis.

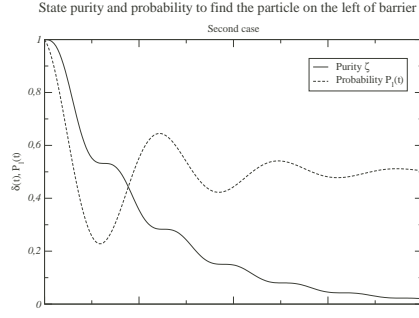


Fig. 4. The tunnelling system coupled to the σ_x reservoir: purity $\zeta(t)$ and probability $P_l(t)$ as a function of time, when the particle is initially prepared in the left side of the potential well, for $k_2 = 1$ and $\omega = 10$. One clearly notes two distinct dynamics in the purity. The plateaux occur at moments in which the system is at one side of the potential well (near integer and half-integer tunnelling periods).

$$\begin{aligned}
 \dot{S}_x &= \omega S_y, \\
 \dot{S}_y &= -2k_2 S_y - \omega S_x, \\
 \dot{S}_z &= -2k_2 S_z.
 \end{aligned} \tag{13}$$

The solution to equation (12) is:

$$\rho(t) = \frac{1}{2} \begin{pmatrix} 1 + e^{-2k_2 t} \cos \theta & c^*(t) \\ c(t) & 1 - e^{-2k_2 t} \cos \theta \end{pmatrix}, \tag{14}$$

with

$$c(t) = e^{(-k_2 t)} \sin(\theta) \left\{ \exp(-i\phi) \cos \epsilon t + \frac{\sin \epsilon t}{\epsilon} [k_2 \exp(i\phi) - i\omega \exp(-i\phi)] \right\},$$

where $\epsilon^2 = \omega^2 - k_2^2$. Again, the interaction with the reservoir destroys the coherence in the initial quantum state, which is transformed into a complete statistical mixture for $k_2 t \gg 1$. As before, the asymptotic state is also localized in the classical statistical sense. However, since the spin flip reservoir acts exactly by random population transfer, the final state presents equal populations on both sides of the barrier, independently of the initial state.

If the system is initially prepared in state $|+x\rangle$ ($\theta = \pi/2$ and $\phi = 0$), once it evolves in time, the particle will tunnel through the barrier and the probability to find it on the left side, will be given by

$$P_l(t) = \frac{1}{2} \left(1 + e^{-k_2 t} \right) \left(\cos \epsilon t + \frac{k_2}{\epsilon} \sin \epsilon t \right), \quad (15)$$

and the purity ζ of the system evolves in time according to

$$\zeta(t) = |c(t)|^2 + e^{-4k_2 t} \cos^2 \theta. \quad (16)$$

In figure 4 one clearly notes two different dynamics in the time evolution of the purity of the quantum state of the particle. When the state of the particle is more localized at one of the sides, the particle loses purity in a much slower rate, while when the particle is tunnelling through the barrier its quantum state loses purity in a faster rate. This behavior is indeed expected given that the particle's position wave function feels the fluctuations of the barrier much strongly when crossing it.

In this case, the Bloch vector picture is subtler. Again, the isolated system would rotate around the O_z axis, but now the fluctuations vary the axis of the movement. The ensemble spreads to neighbor circles, and the circle plains also fluctuate. In the asymptotic limit ($k_2 t \gg 1$) all points are possible and the Bloch vector tends to the center of the sphere.

With the usual assumption $\omega \gg k_2$, the $|\pm_z\rangle$ states are the most robust states. They can also be classified as pointer states, by the predictability sieve criterion [9], but in a sense different to that of the first case. Here, no vector is rigorously unaffected. The fluctuations induce random rotations around O_x axis so that when the particle is localized on one side of the barrier, its Bloch vector being aligned with O_x , it is *instantaneously* immune to the reservoir. This means that the spin-flip reservoir would tend to keep $|\pm_x\rangle$ states fixed, however the unitary evolution takes them off the O_x axis, and the other vectors that appear in their trajectories are strongly affected by decoherence (see fig. 5).

Finally, we will describe a feasible trapped ions experiment to observe the

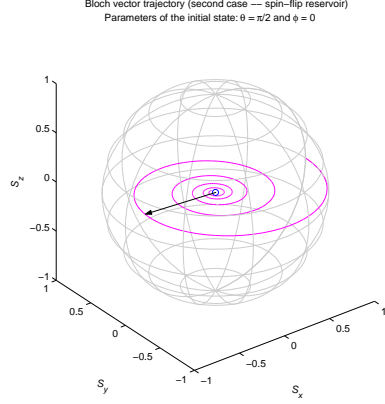


Fig. 5. When the tunnelling system is coupled to a spin-flip reservoir, no Bloch vector remains fixed. Here we show one of the pointer states, aligned with the O_x axis. Even this state is not preserved because it is taken off its original axis by the unitary evolution, making it vulnerable to the reservoir and allowing decoherence to take place.

decoherence effects on double well tunnelling. The basic ingredients are: a single trapped ion, two of its electronic levels, $\{|g\rangle, |e\rangle\}$, and an external laser field of frequency ω_L . The ion is initially prepared in lower level $|g\rangle$ and it is cooled down to its vibrational ground state which, for a harmonic trap, is a gaussian distribution around the center of the trap. The external laser field is then focused to the right of the ionic distribution, and it is largely blue shifted in respect to the ionic $|g\rangle \rightarrow |e\rangle$ transition, i.e. $\Delta = \omega_L - \omega_{eg} \gg G$, where G is the coupling constant of the chosen transition. The dispersive interaction between the ion and the laser beam induces a repulsive dipole optical force in the ion, pushing it away from the focus of the laser field. In fact, this new interaction constitutes an optical potential barrier to the motion of the ion. The laser is then pushed to the left until it reaches the center of the trapping potential, configuring a double well potential for the motion of the ion. If the process is adiabatic, the ion is pushed to the left side of the well and if the laser is intense enough, the ion remains there, i.e. there is no tunnelling to the right side of the trap. If the laser intensity is now reduced, the central barrier is lowered and the ion tunnels through this barrier undergoing Rabi oscillations between the left and right sides of the double well. Fluorescence of the ion can then be used to measure its position in either side of the well for different times. The fluctuations of the dimensions and positions of the barrier can be easily obtained in a controlled way by randomly altering the intensity or the position of the laser beam.

In this letter we used a simple model to show that, for long times, a quantum system, able to undergo tunnelling between two potential wells, coupled to dissipative reservoirs tends to localize. We also suggested a simple experiment with trapped ions to observe this effect.

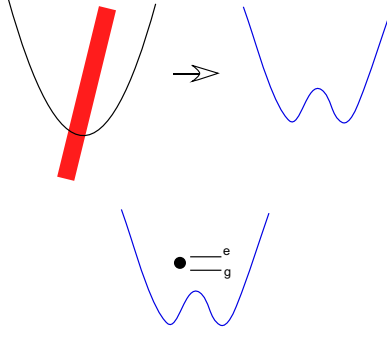


Fig. 6. A schematic draft of an ion trap traversed by an external laser field forming a double potential well.

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